R & D facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Chemistry and Surface Science

08/2008

Nano-Materials and Catalyst Research Laboratory

Materials and catalysts are essential to progress in any number of energy-related applications. The Materials and Catalyst Research Laboratory is well equipped to address a wide range of scientific questions about novel concepts. The laboratory takes on a wide span of work from synthesis and characterization of novel catalysts and adsorbents to investigation of their properties with an array of basic surface-science techniques. The scope of materials under investigation is also wide. New microporous materials called Metal Organic Frameworks (MOFs) are designed, synthesized, and evaluated for their ability to adsorb and separate gases, including the separation of carbon dioxide. Critical parameters such as surface area, low temperature, high resolution isotherms, and isosteric heats of adsorption are obtained with a state-of-the-art instrument. Isotherms over a wider range of pressure (0–80 atm) and temperature are taken with a specially designed instrument. Spectroscopic methods are used to provide more detailed information about the adsorption sites. Direct observations of adsorbed gases are made with either an infrared or a Raman instrument. A specially designed and constructed variable-temperature, variable-pressure view cell provides a unique method to obtain critical information on the specific sites responsible for adsorption.

Versatile surface science instrument for fundamental studies of catalysts.

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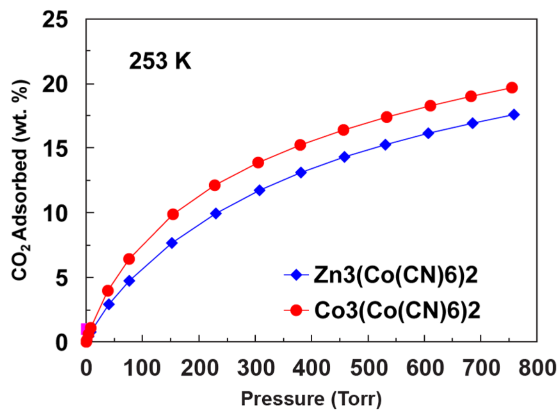
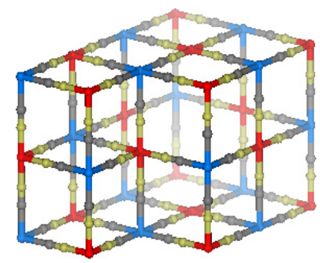
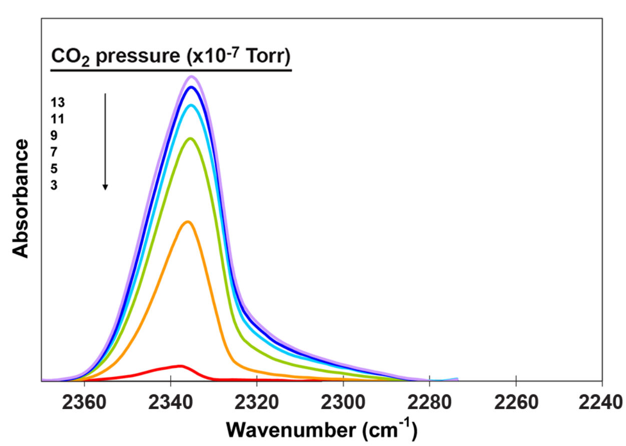
The infrared bands of adsorbed gases are often shifted according to the nature of the sites they occupy. Information on the relative binding strength of the sites is obtained from competition experiments in which one gas is displaced by another. The experimental results are compared with computer simulations to shed more light on the energy of the solid/gas interactions and their spatial aspects.





Fundamental investigations of the surface science of novel catalysts are carried out with a versatile instrument equipped with wide variety of techniques including XPS, LEED, Ion Scattering and Auger, AMF, and STM. Well defined surfaces may be coated with other metals by an in-situ evaporator. This powerful instrument is used to study the basic chemistry of the surfaces of the numerous catalysts used in Fischer-Tropsch synthesis, alcohol synthesis, and other fuel-related processes. The relationships between catalytic activity and the size, shape, or the exposed facet of crystalline particles are key points of interest. The development of new techniques to synthesize nano-scale catalyst particles with predetermined sizes, shapes, and crystalline facets inspires this work. The combination of controlled synthesis and surface-science experiments offers a potent means to develop catalysts with both higher activity and selectivity. Loss of activity due to sintering is a perennial problem associated with catalysts of very small particle sizes. One method to overcome this problem is to encapsulate the catalyst particle in a protective coating. This must be done without appreciable loss of the ability of the reactants to reach the catalyst surface. Surface science techniques are playing a vital role in the characterization of such novel catalytic systems.



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